AN 2002:214480 CAPLUS
DN 136:377729
TI Novel high birefringence dibenzothiophenylacetylene liquid crystals
AU Sekine, Chizu; Ishitobi, Masamitsu; Iwakura, Kazunori; Minai, Masayoshi; Fujisawa, Koichi
CS Tsukuba Research Laboratory, Sumitomo Chemical Co. Ltd., Tsukuba, 300-3294, Japan
SO Liquid Crystals (2002), 29(3), 355-367
CODEN: LICRE6; ISSN: 0267-8292
PB Taylor & Francis Ltd.
DT Journal
LA English
CC 75-11 (Crystallography and Liquid Crystals)
Section cross-reference(s): 27, 73, 74
AB The authors have designed, synthesized and evaluated dibenzothiophenylacetylene homologs as new heterocyclic mols. which were expected to have high .DELTA..alpha. values and short wavelength UV absorption spectra. The dibenzothiophenyl acetylene homologs exhibited wide nematic phase ranges and had very high extrapolated .DELTA.n of over 0.6 and directly measured values of 0.5. The compds. with two dibenzothiophenyl rings were colorless, so that the authors have succeeded in obtaining colorless super-high .DELTA.n liq. crystals. The authors also analyzed the contribution of the transition band to the refractive indexes and the birefringence. From the anal., the main origins of .DELTA.n for compds. 1 and 2 are lower MOs than the HOMO and this results in the compatibility of large .DELTA.n and lack of color. The dibenzothiophenylacetylene compds. behaved according to the authors' design expectations.
ST birefringence dibenzothiophenylacetylene deriv liq crystal prepn property
IT Liquid crystals
(design, synthesis, and mesomorphic and optical properties of high-birefringence dibenzothiophenylacetylene derivs.)
IT Birefringence
UV and visible spectra
(of dibenzothiophenylacetylene deriv. liq. crystals)
IT Polarizability
Refractive index
(of high-birefringence dibenzothiophenylacetylene derivs.)
IT Liquid crystals
(transitions; of high-birefringence dibenzothiophenylacetylene derivs.)
IT 425404-03-1P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn. and (hexylidene)dibenzothiophenylacetylene)
IT 25288-76-0P, 3-Dibenzothiophenamine
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn. and bromination of)
IT 425404-07-5P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn. and desilylation of)
IT 425404-00-8P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn. and esterification of)
IT 1013-23-6P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn. and nitric acid reaction with)
IT 425403-99-2P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn. and oxidn. of)

IT 425403-94-7P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn. and reaction dibenzothiophenylacetylene(ethylphenyl trifluorosulfonate))
IT 425403-93-6P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn. and reaction potassium hydroxide in toluene)
IT 425403-96-9P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn. and reaction with dibenzothiophenylacetylene and pentyloxyphenylacetylene)
IT 425404-04-2P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn. and reaction with hexyne and phenyldioxoborane)
IT 425403-97-0P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn. and reaction with nitric acid)
IT 425404-08-6P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn. and reaction with pentyloxydibenzothiophenylacetylene(ethylphenyl trifluorosulfonate))
IT 97511-04-1P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn. and reaction with propargyl alc. in presence of palladium dichloride, triphenylphosphine and triethylamine in Et acetate)
IT 425404-01-9P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn. and reaction with triethylamine and toluenesulfonic acid in methanol)
IT 425403-95-8P 425404-02-0P 425404-05-3P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn. and reaction with trifluoromethanesulfonic anhydride)
IT 425404-06-4P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn. and reaction with trimethylsilylacetylene)
IT 68925-98-4P 425403-98-1P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn. and redn. of)
IT **425403-90-3P 425403-91-4P 425403-92-5P**
RL: PEP (Physical, engineering or chemical process); PRP (Properties); PYP (Physical process); SPN (Synthetic preparation); PREP (Preparation); PROC (Process)
(prepn., liq. crystal properties and optical properties of)
IT 67589-39-3, 4-Ethoxyphenyl trans-4-propylcyclohexylcarboxylate
67589-41-7, 4-Butoxyphenyl trans-4-propylcyclohexylcarboxylate
67589-47-3, 4-Ethoxyphenyl trans-4-butylcyclohexylcarboxylate
67589-52-0, 4-Methoxyphenyl trans-4-pentylcyclohexylcarboxylate
67589-53-1, 4-Ethoxyphenyl trans-4-pentylcyclohexylcarboxylate
RL: NUU (Other use, unclassified); PRP (Properties); USES (Uses)
(refractive indexes and dichroic ratios of polarized UV spectra of dibenzothiophenylacetylene derivs. in liq. crystal mixt. contg.)
RE.CNT 24 THERE ARE 24 CITED REFERENCES AVAILABLE FOR THIS RECORD
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(5) Fontana, M; Phys Rev A 1986, V33, P4132 CAPLUS
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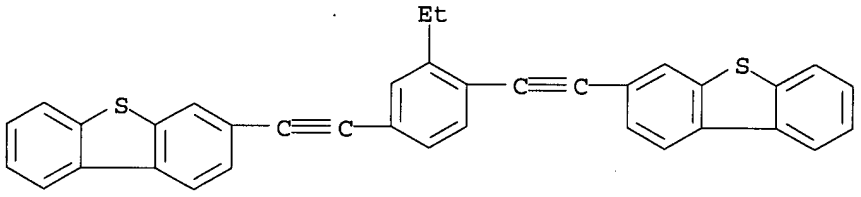
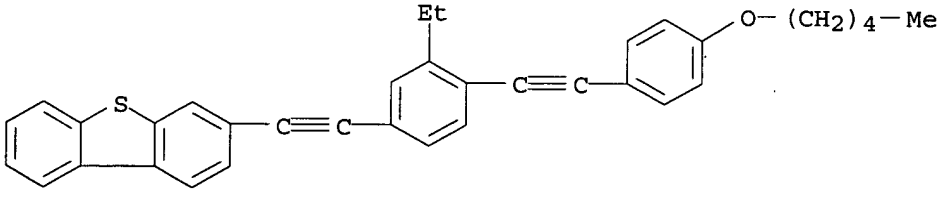
(19) Vuks, M; Opt Spektrosk 1996, V20, P644
(20) Wu, S; J appl Phys 1989, V65, P4372 CAPLUS
(21) Wu, S; J appl Phys 1991, V69, P2080 CAPLUS
(22) Wu, S; Phys Rev A 1986, V33, P1270 CAPLUS
(23) Wu, S; SID 2001 Dig 2001, P954 CAPLUS
(24) Wu, S; SID Tech Dig 1985, V16, P262

IT **425403-90-3P 425403-91-4P 425403-92-5P**
RL: PEP (Physical, engineering or chemical process); PRP (Properties); PYP (Physical process); SPN (Synthetic preparation); PREP (Preparation); PROC (Process)
(prepn., liq. crystal properties and optical properties of)

RN 425403-90-3 CAPLUS
CN Dibenzothiophene, 3,3'-[(2-ethyl-1,4-phenylene)di-2,1-ethynediyl]bis- (9CI) (CA INDEX NAME)



RN 425403-91-4 CAPLUS
CN Dibenzothiophene, 3-[[3-ethyl-4-[[4-(pentyloxy)phenyl]ethynyl]phenyl]ethynyl]- (9CI) (CA INDEX NAME)



RN 425403-92-5 CAPLUS
CN Dibenzothiophene, 3-[[3-ethyl-4-[[7-(1E)-1-hexenyl-3-dibenzothienyl]ethynyl]phenyl]ethynyl]-7-(pentyloxy)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

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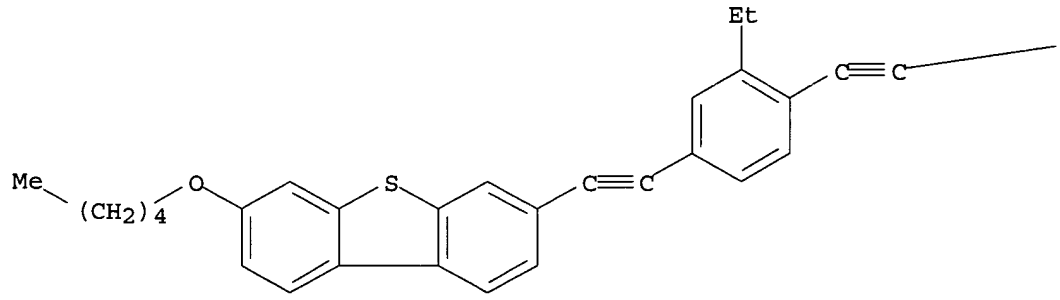

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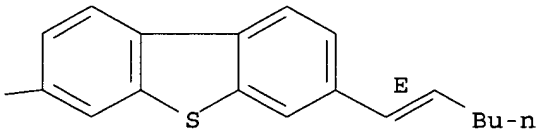

AN 2002:616226 CAPLUS
DN 137:177210
TI Compound having phenylacetylene structure, liquid crystal composition, polymer, optically anisotropic product, optical or liquid crystal element, dibenzothiophene compound, intermediate, and process for producing the same
IN Sekine, Chizu; Ishitobi, Masamitsu; Fujisawa, Koichi; Iwakura, Kazunori; Minai, Masayoshi
PA Japan
SO U.S. Pat. Appl. Publ., 74 pp.
CODEN: USXXCO
DT Patent
LA English
IC ICM C09K019-52
ICS C09K019-30; C07C025-13; C07D495-00; C07D335-10
NCL 428001100
CC 74-13 (Radiation Chemistry, Photochemistry, and Photographic and Other Reprographic Processes)
Section cross-reference(s): 75
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	US 2002110650	A1	20020815	US 2002-67871	20020208
	JP 2002255960	A2	20020911	JP 2001-52954	20010227
	JP 2002322174	A2	20021108	JP 2002-24353	20020131
	JP 2002322215	A2	20021108	JP 2002-24425	20020131
	GB 2380192	A1	20030402	GB 2002-2907	20020207
	DE 10205367	A1	20021212	DE 2002-10205367	20020208
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OS MARPAT 137:177210
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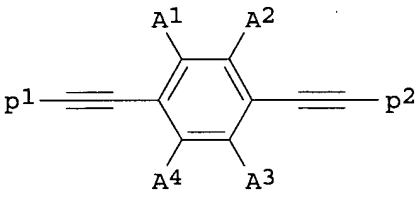

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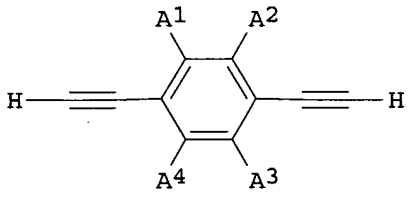


II

AB The present invention relates to liq. crystal compns., polymers, optically anisotropic products, and optical or liq. crystal elements that have large refractive index anisotropy, mix easily with other liq. crystals, have advantageous stability against light, and exhibit absorption at practically short wavelength in the UV region. The present invention also relates to phenylacetylene structure compds. which are useful as optical display, and recording materials, as optical compensators, polarizer materials, reflector plates, etc., all for liq. crystal display devices. The compds. are represented by I (A1-4 = H, F, C1-10 alkyl or alkoxy

optionally substituted with F; P1,2 = structure fulfilling the conditions of HOMO energy and polarizability) and have a phenylacetylene structure, wherein difference .DELTA.E in energy of HOMO of parts II, P1-H and P2-H calcd. by the method of MOs is .gtoreq. 0.3 eV, and the polarizability anisotropy .DELTA..alpha. of a mol. represented by I calcd. in the same way is .gtoreq. 500 A.U.

ST liq crystal display phenylacetylene dibenzothiophene compd

IT Liquid crystals
(Compd. having phenylacetylene structure and dibenzothiophene compd. for liq. crystal compn. for)

IT **425403-90-3P 425403-91-4P 446023-58-1P**
RL: PRP (Properties); SPN (Synthetic preparation); TEM (Technical or engineered material use); PREP (Preparation); USES (Uses)
(compd. having phenylacetylene structure and dibenzothiophene compd. for liq. crystal display)

IT 379268-41-4P
RL: SPN (Synthetic preparation); TEM (Technical or engineered material use); PREP (Preparation); USES (Uses)
(compd. having phenylacetylene structure and dibenzothiophene compd. for liq. crystal display)

IT 224648-09-3 239104-43-9 239104-50-8 251467-52-4 296255-72-6 299411-32-8 299411-39-5 446023-47-8 446023-48-9
RL: TEM (Technical or engineered material use); USES (Uses)
(liq. crystal compn.; compd. having phenylacetylene structure and dibenzothiophene compd. for liq. crystal display)

IT 425403-94-7P 425403-96-9P 425404-00-8P 425404-01-9P 425404-03-1P 446023-43-4P 446023-45-6P
RL: PRP (Properties); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn. of compd. having phenylacetylene structure and dibenzothiophene compd. for liq. crystal display)

IT **446023-46-7P**
RL: PRP (Properties); SPN (Synthetic preparation); TEM (Technical or engineered material use); PREP (Preparation); USES (Uses)
(prepn. of compd. having phenylacetylene structure and dibenzothiophene compd. for liq. crystal display)

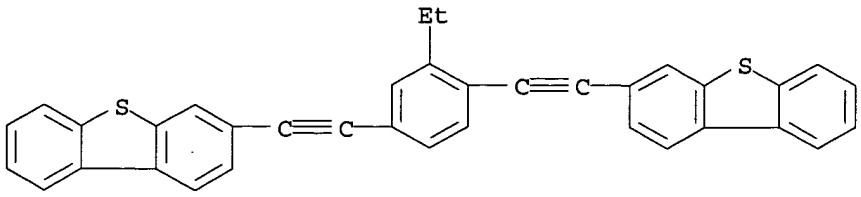
IT 110-87-2, Dihydropyran 115-19-5, 2-Methyl-3-butyne-2-ol 132-65-0, Dibenzothiophene 274-07-7, Catecholborane 628-17-1, 1-Iodopentane 693-02-7, 1-Hexyne 814-68-6, Acrylic acid chloride 4286-55-9 50816-19-8, 8-Bromo-octanol 79887-16-4 350036-14-5
RL: RCT (Reactant); RACT (Reactant or reagent)
(prepn. of compd. having phenylacetylene structure and dibenzothiophene compd. for liq. crystal display)

IT 1013-23-6P 25288-76-0P, 3-Dibenzothiophenamine 56554-20-2P 68925-98-4P 97511-04-1P 425403-95-8P 425403-97-0P 425403-98-1P 425403-99-2P 425404-02-0P 425404-04-2P 446023-40-1P 446023-41-2P 446023-42-3P 446023-44-5P 446023-49-0P 446023-50-3P 446023-51-4P 446023-52-5P 446023-53-6P 446023-54-7P 446023-55-8P **446023-56-9P 446023-57-0P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn. of compd. having phenylacetylene structure and dibenzothiophene compd. for liq. crystal display)

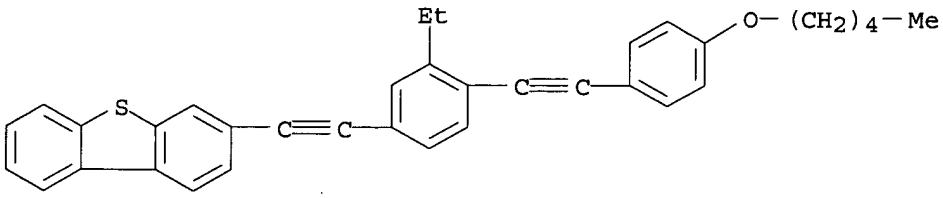
IT **425403-90-3P 425403-91-4P 446023-58-1P**
RL: PRP (Properties); SPN (Synthetic preparation); TEM (Technical or engineered material use); PREP (Preparation); USES (Uses)
(compd. having phenylacetylene structure and dibenzothiophene compd. for liq. crystal display)

RN 425403-90-3 CAPLUS

CN Dibenzothiophene, 3,3'-[(2-ethyl-1,4-phenylene)di-2,1-ethynediyl]bis- (9CI) (CA INDEX NAME)

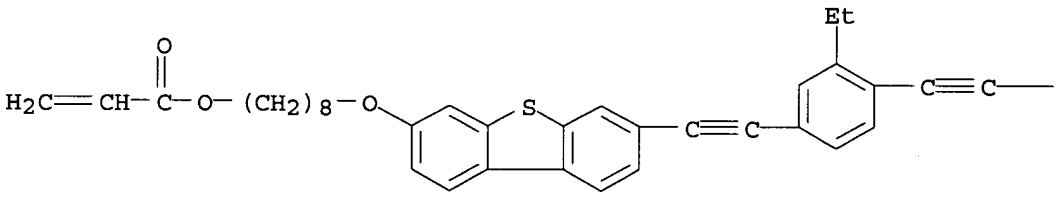


RN 425403-91-4 CAPLUS
CN Dibenzothiophene, 3-[[3-ethyl-4-[[4-(pentyloxy)phenyl]ethynyl]phenyl]ethynyl]- (9CI) (CA INDEX NAME)



RN 446023-58-1 CAPLUS
CN 2-Propenoic acid, 8-[[7-[[3-ethyl-4-[[7-[[6-[(1-oxo-2-propenyl)oxy]hexyl]oxy]-3-dibenzothienyl]ethynyl]phenyl]ethynyl]-3-dibenzothienyl]oxy]octyl ester (9CI) (CA INDEX NAME)

PAGE 1-A



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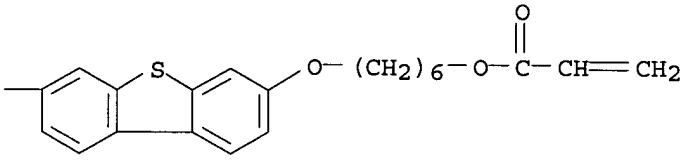
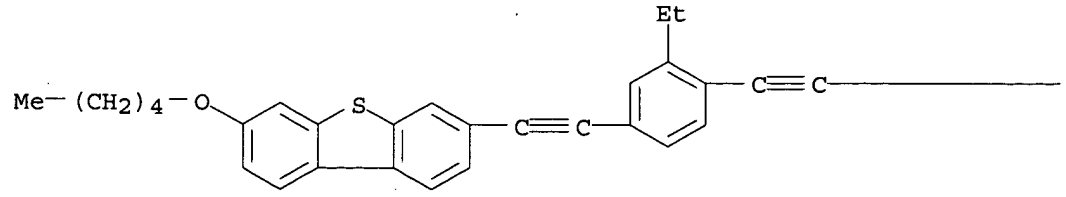


IT **446023-46-7P**
RL: PRP (Properties); SPN (Synthetic preparation); TEM (Technical or engineered material use); PREP (Preparation); USES (Uses)
(prepn. of compd. having phenylacetylene structure and dibenzothiophene compd. for liq. crystal display)
RN 446023-46-7 CAPLUS
CN Dibenzothiophene, 3-[[3-ethyl-4-[[7-(1-hexenyl)-3-dibenzothienyl]ethynyl]phenyl]ethynyl]-7-(pentyloxy)- (9CI) (CA INDEX NAME)

PAGE 1-A



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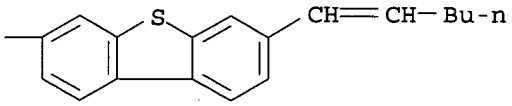
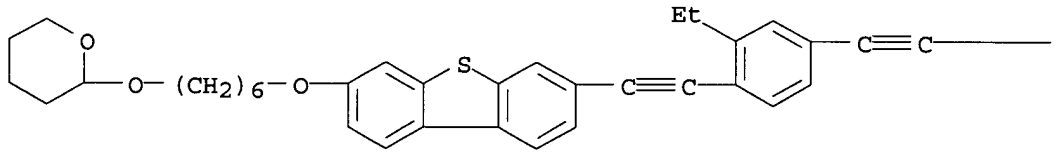


IT **446023-56-9P 446023-57-0P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn. of compd. having phenylacetylene structure and dibenzothiophene compd. for liq. crystal display)

RN 446023-56-9 CAPLUS

CN 1-Octanol, 8-[[7-[[3-ethyl-4-[[7-[[6-[(tetrahydro-2H-pyran-2-yl)oxy]hexyl]oxy]-3-dibenzothienyl]ethynyl]phenyl]ethynyl]-3-dibenzothienyl]oxy]-, acetate (9CI) (CA INDEX NAME)

PAGE 1-A



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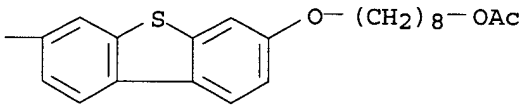
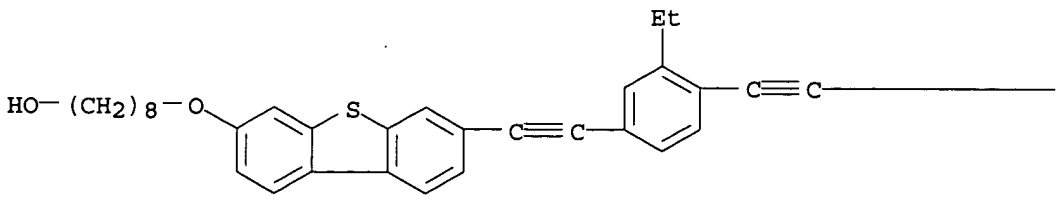


RN 446023-57-0 CAPLUS

CN 1-Octanol, 8-[[7-[[3-ethyl-4-[[7-[(6-hydroxyhexyl)oxy]-3-dibenzothienyl]ethynyl]phenyl]ethynyl]-3-dibenzothienyl]oxy]- (9CI) (CA INDEX NAME)

PAGE 1-A



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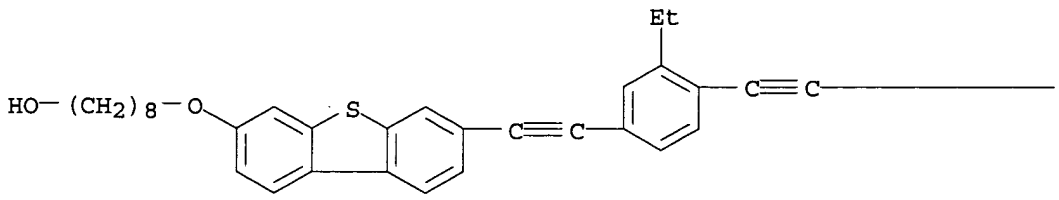

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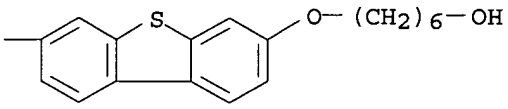

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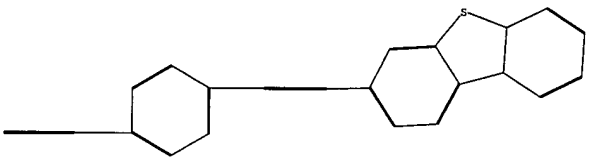

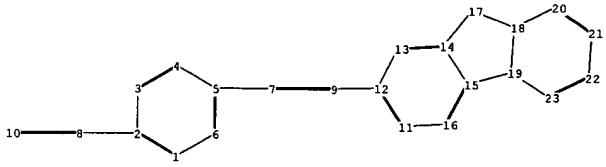

chain nodes :
7 8 9 10
ring nodes :
1 2 3 4 5 6 11 12 13 14 15 16 17 18 19 20 21 22 23
chain bonds :
2-8 5-7 7-9 8-10 9-12
ring bonds :
1-2 1-6 2-3 3-4 4-5 5-6 11-12 11-16 12-13 13-14 14-15 14-17 15-16 15-19
17-18 18-19 18-20 19-23 20-21 21-22 22-23
exact/norm bonds :
14-17 15-19 17-18 18-19 18-20 19-23 20-21 21-22 22-23
exact bonds :
2-8 5-7 7-9 8-10 9-12
normalized bonds :
1-2 1-6 2-3 3-4 4-5 5-6 11-12 11-16 12-13 13-14 14-15 15-16

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS 8:CLASS 9:CLASS 10:CLASS
11:Atom 12:Atom 13:Atom 14:Atom 15:Atom 16:Atom 17:Atom 18:Atom 19:Atom 20:Atom
21:Atom 22:Atom 23:Atom